New Insights into the Born Oppenheimer Approximation and "Potential Effects" with No Ordinary Potentials

T. Kaufherr[1,3], Y. Aharonov[1,2], S. Nussinov[1], J. Tollaksen[2]

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(1)Tel Aviv University, School of Physics and Astronomy, Tel Aviv 69978, Israel
(2)Chapman University, Schmid College of Sciences, Orange, CA 92866, USA
(3)E-mail: trka@post.tau.ac.il

Abstract

The present article addresses a novel possibility of having, within the Born Oppenheimer set-up, a shift of the interference pattern of the external heavy particle. We carefully engineer a gedanken experimental set-up in which such a shift occurs, in spite of the fact that any experiment, utilizing a weakly interacting test particle designed to monitor the system, records no force and no potential. Thus we have effectively generated in this particular adiabatic context an "Effect of Electromagnetic Potentials" even though no such potentials exist.

I. Introduction

In a previous paper [1] we introduced, in the context of a one dimensional scattering problem, the concepts of "potential", virtual forces and private potentials. In the present work we discuss at some length these concepts in their most natural setting which is the Born Oppenheimer approximation [2]. Using a strongly rather than a weakly interacting particle highlights another key aspect of the nontrivial Born Oppenheimer set-ups, in addition to the adiabaticity. Specifically, it is that the external particle can in fact modify the system with which it interacts.

We consider a "strong" version of the electric Aharonov Bohm[AB] Effect [1, 3]. Rather than having a weakly interacting external particle (i.e; an electron) which does not change the separation between the condenser plates, here we have a strongly interacting, heavy external particle, which

does polarize the atom with which it interacts. The set-up considered is the following: a polarizable atom (dipole) which is viewed as a two-level system, is located at the origin. The external particle is prepared in a superposition of two wave packets. The interaction with the dipole is then adiabatically turned on. After some finite time interval the interaction is again adiabatically turned off. We calculate the relative phase acquired between the two wave packets of the external particle. We next find that this relative phase depends on "potential" virtual forces that would have acted on the external particle at locations between the two wave packets. These forces derive from an appropriate "private", Born Oppenheimer, potential.

Finally, an appropriately tuned set-up of two dipoles can generate non-trivial private potentials (forces) in an entirely standard, "public" force-free environment. The resulting shift of the interference pattern of the external heavy particle is therefore observable in this set-up, even when no ordinary public potentials exist. Thus using the terminology of the original AB paper, we have here a phenomenon akin to the electromagnetic potentials effect but without any potentials.

II. The Born-Oppenheimer Approximation

We consider a two-level system, represented here by an electric dipole whose positive charge is fixed at the origin. Let the Pauli matrices $\sigma_1, \sigma_2, \sigma_3$, operate on the Hilbert space of our two-level system. Using these matrices we construct the electric dipole operator $\vec{d} = ed\vec{\sigma} = ed(\sigma_1\hat{x} + \sigma_2\hat{y} + \sigma_3\hat{z})$. An external, heavy, charged particle of charge Q, moving along the positive z axis interacts strongly with the dipole. The interaction is $Q\frac{\vec{d}\cdot\hat{r}}{r^2} = \frac{Qe\sigma_3}{z^2} \equiv \sigma_3 f(z)$ where we have approximated the separation $\vec{r} \approx \vec{r}_{ext} = \vec{z}$. For a given position z of the external particle, the dipole's Hamiltonian is

$$H_1 = \alpha\sigma_1 + g(t)f(z)\sigma_3 \equiv H_F + V(z,t)\,, \tag{1}$$

with $g(t)$ a slowly varying adiabatically on and off switching function such that $g(-\infty) = g(+\infty) = 0$. The total Hamiltonian of the system is

$$H = \frac{p^2}{2M} + H_1 \tag{2}$$

where $p = \frac{1}{i}\frac{\partial}{\partial z}$ is the external particle's momentum and M is its mass. Initially, at $t = -\infty$, the dipole is closed, i.e., $g(-\infty) = 0$. At that time, the dipole is in its ground state: $\phi(-\infty) = \phi_g = |\sigma_1 = -1>$. Hence the initial state is unpolarized, namely $\bar{\sigma}_3(-\infty) = 0$. The ground state energy is $E_g(-\infty) = -\alpha$. The other eigenstate is $\phi_{exc} = |\sigma_1 = +1>$ with an energy gap of 2α between the states. The stage is set when the external particle is prepared to be at rest in a coherent superposition $\Psi_{xp} = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$,

$\psi_i = \psi[z - z(i)]$, such that ψ_1 is, effectively, outside the range of the interaction. The two wave packets are enclosed in small spherical Faraday cages centered at $z(1)$, $z(2)$, respectively, with the cage containing ψ_1 being grounded. This then ensures that there is no interaction between the dipole and the external particle when in ψ_1. See fig.1. The interaction is now turned on adiabatically, until g(t) reaches at t_1 its maximal value $g(t_1) \equiv g(0)$ such that $g(0)f[z(2)] \sim \alpha$. The adiabaticity ensures that the dipole remains in its instantaneous ground state $\phi_g(z,t)$ throughout, and that the ground state energy changes according to $E_g(z,t) = -\sqrt{\alpha^2 + g^2(t)f^2(z)}$ [4]. In addition, the dipole becomes polarized [5],

$$\bar{\sigma}_3(z,t) =< \phi_g \mid \sigma_3 \mid \phi_g >= \frac{-g(t)f(z)}{\sqrt{\alpha^2 + g^2 f^2}} \,. \tag{3}$$

When the external particle is in ψ_1 the dipole vanishes, while if it is in ψ_2, a finite dipole moment is induced. Thus the external particle and the dipole become entangled. We now proceed to solve for the time evolution of the external particle. In the Born Oppenheimer approximation one assumes that the light degree of freedom is in an eigenstate of energy. Thus, with the dipole prepared in the ground state of its free Hamiltonian and the adiabatic turning on of the interaction, the Born Oppenheimer approximation is applicable. The effective Hamiltonian of the external particle is then given by

$$H_{eff} = \frac{p^2}{2M} + E_g(z,t) \tag{4}$$

The single valuedness of $E_g(z,t)$ in the adiabatic "limit" guarantees that it is a bona-fide potential function. When M$\rightarrow \infty$ and the kinetic energy of the external particle is neglected, the state of the system reads

$$\Psi(t) = \frac{1}{\sqrt{2}} \left[\psi_1 \mid E_1 > e^{-i\int_{-\infty}^{t} E_1(t')dt'} + \psi_2 \mid E_2 > e^{-i\int_{-\infty}^{t} E_2(t')dt'} \right] , \tag{5}$$

where $E_i(t) \equiv E_g[z(i),t]$, $\mid E_i > \equiv \mid E_g[z(i),-\infty] >$.

We would like now to calculate the Born Oppenheimer potential difference $E_g[z(2),t] - E_g[z(1),t] \equiv E_2(t) - E_1(t)$ seen by the external particle by integrating the forces acting on it. Consider the Hamiltonian(1). Note that z, the position of the external particle, is here a parameter. Using stationary state perturbation theory to calculate the change in the dipole's ground state energy, we obtain [6]

$$E_g[z(2),t] - E_g[z(1),t] = g(t) \int_{z(1)}^{z(2)} \frac{\partial f}{\partial z} \bar{\sigma}_3(z) dz = - \int_{z(1)}^{z(2)} \bar{F} dz \,. \tag{6}$$

Equation (6) connects the single particle, as described by the Born Oppenheimer approximation, with the underling particle$\oplus$dipole description. It

states that the Born Oppenheimer force $F_{BO} = -\frac{\partial E_g}{\partial z}$ equals $-g(t)\bar{\sigma}_3(z)\frac{\partial f}{\partial z}$. This is a private force since the dipole's polarization, generating the force, depends on the external particle's position. With the external particle in ψ_1, ψ_2, the forces appearing on the rhs of (6) are *virtual* forces, namely, forces that would have acted on the external particle had it been placed in intermediate points, between $z(1)$ and $z(2)$. We have thus shown, within the Born Oppenheimer approximation, that the private potential difference between $z(2)$ and $z(1)$ equals to the corresponding path integral of private, "virtual" forces. In other words, we have here an electric AB type effect, with the Born Oppenheimer or private potential replacing the public potential and the private forces replacing the ordinary, public forces. The public forces (potentials) are the ordinary concepts, defined by using infinitesimal test particles. Such weakly interacting particles do not modify the system with which they interact.

Using equations (5) and (6) we find that the Born Oppenheimer potential difference introduces a relative phase between the external particle's two wave packets that is given by

$$\varphi_{rel}(t) = \int_{z(1)}^{z(2)} \int_{-\infty}^{t} \bar{F} dz dt \, . \tag{7}$$

We shall next sketch an interference experiment measuring this phase. Having prepared the system as described above, see also fig.[2], the external heavy particle (which is now in a superposition of two wavepackets ψ_1 and ψ_2) keeps having a constant interaction with the dipole for a finite time interval $[t_1, t_2]$, after which it is adiabatically switched off. Specifically, let

$$g(t) = \begin{cases} g(0)e^{\varepsilon(t-t_1)} & t \le t_1 < 0 \\ g(0) & t_1 \le t \le t_2 \\ g(0)e^{-\varepsilon(t-t_2)} & t \ge t_2 > 0 \, . \end{cases} \tag{8}$$

Clearly, in the experimental set-up (fig. 2) we do not use infinite switching on and off times T. Having $e^{-\varepsilon|T|} \ll 1$ suffices to justify the formal infinite time integrations below. (See also the discussion in section III.) The single valuedness of the adiabatic limit guarantees that the system disentangles as $g(t)$ is turned off. Specifically,

$$\Psi(t \ge t_2) = |\sigma_1 = -1 > \frac{1}{\sqrt{2}}(\psi_1 + e^{i\varphi_{rel}(t_2)}\psi_2) \, , \tag{9}$$

$$\varphi_{rel}(t_2) = \int_{t_1}^{t_2} \{E_g[z(2), t] - E_g[z(1), t]\} \, dt \tag{10}$$

$$= \left[\sqrt{\alpha^2 + g^2(0) f^2[z(2)]} - \alpha\right](t_2 - t_1) \, , \tag{11}$$

where we have ignored the relative phase accumulated during the opening and closing time. The two wavepackets, brought back to $z(0)$, halfway between

$z(1)$ and $z(2)$, will then interfere. Sending N similarly prepared particles past the dipole, repeating the steps described above each time, the shift in the interference pattern becomes observable and $(6, 11)$ should be confirmed. Note that both wave packets, being enclosed in Faraday cages, are confined to (private) force-free regions throughout the experiment.

We will now show that by replacing the above single dipole by *two* properly tuned dipoles we can make the public forces and potentials vanish everywhere. Yet the private potential difference and the ensuing relative phase do *not* vanish. The Hamiltonian now becomes,

$$H_1 + H_2 = \alpha_1 \sigma_1^1 + \beta_1 g(t) f(z) \sigma_3^1 + \alpha_2 \sigma_1^2 + \beta_2 g(t) f(z) \sigma_3^2 \,. \tag{12}$$

Dipole #1 is initially prepared to be in the ground state, namely the state $| \sigma_1 = -1 >$, while dipole #2 is prepared in the excited state, $| \sigma_1 = +1 >$. Thus the dipoles' polarizations are reversed. This implies that it is possible to make the public potential and force vanish everywhere, by choosing $\beta_1 \bar{\sigma}_3^1 + \beta_2 \bar{\sigma}_3^2 = 0$ [7]. But there still is a nonvanishing private or Born Oppenheimer potential difference between the Faraday cages [7] which will produce a phase shift. This phase shift will manifest in the interference pattern.

For the sake of simplicity we have omitted in the Hamiltonian (12) the Coulomb interaction between the two dipoles. In the present framework this interaction, which disfavours the state when the two dipoles are parallel, is modeled by an additional interaction term $\beta \sigma_3^1 \sigma_3^2$. The full Hamiltonian is $H = \alpha_1 \sigma_1^1 + \alpha_2 \sigma_1^2 + \beta \sigma_3^1 \sigma_3^2 + \gamma_1 \sigma_3^1 + \gamma_2 \sigma_3^2$. Roughly speaking, since the coupling term enhances reversed polarization, the condition for the vanishing of the public potential, i.e; $\gamma_1 \sigma_3^1 + \gamma_2 \sigma_3^2 \equiv 0$, can be readily met in this more realistic case as well. The detailed calculation may be discussed in the future.

III. Summary and Conclusions

our discussion so far has been largely conceptual. We now briefly address the feasibility of the experiments described above. In order to achieve an effective two-level system, a very small splitting between the ground state and the first excited state, as compared with all other energy differences of the system, is required.

In the present electric dipole context we model the "polarizable atom" by a single electron (or ion) which tunnels between two small conducting regions (or traps). The distance d between these regions is much larger than their size r. In this essentially double-well system the ground state (excited state) of the electron is the symmetric (antisymmetric) superpostion $\frac{1}{\sqrt{2}}(\psi_L \pm \psi_R)$ respectively, where ψ_L (ψ_R) refers to the electron being in the ground state of the left (right) potential well. The splitting between the two levels (2α

in our terminology) is thus rather small. Hence also our requirement that the interaction strength with the external particle be of order of α which determines the splitting can be readily met with no additional demand on the size of its charge.

To verify the applicability of the adiabatic approximation in the two-level system sketched above, we use the following qualitative argument. Let $r \approx \mathrm{O}(100\ \mathring{A})$ and $d \approx \mathrm{O}(1000\ \mathring{A})$. The choice of r implies that the first excited state of the sigle electron in each of the circular patches separately is

$$\frac{\hbar^2}{2m_e r^2} \sim \frac{1}{100} eV \sim 10^{13} sec^{-1} \tag{13}$$

above the ground state. On the other hand, the splitting 2α in the double well, which is proportional to the tunneling frequency ω_t, is vastly smaller than (13). This last frequency critically depends on the distance between the patches and can be tuned to a desired, sufficiently large, value. Specifically, we use this to ensure the adiabaticiy condition $\mathrm{T}\omega_t \gg 1$ where T is the duration of the interference experiment.

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[4] $H_1^2 = \alpha^2 + g^2(t) f^2(z)$ having used $\sigma_i^2 = 1$ and $[\sigma_i, \sigma_j]_+ = 0$.

[5] With $\alpha \equiv \lambda_1$, $g(t)f(z) \equiv \lambda_2$, the stationary Schrödinger equation for the groundstate is

$$\begin{pmatrix} \lambda_2 & \lambda_1 \\ \lambda_1 & -\lambda_2 \end{pmatrix} \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} = -|E| \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} .$$

We obtain $\bar{\sigma}_3 = \cos^2\theta - \sin^2\theta = -\frac{\lambda_2}{|E|} = -\frac{\lambda_2}{\sqrt{\lambda_1^2+\lambda_2^2}}$. For the excited state $\bar{\sigma}_3 = \frac{\lambda_2}{|E|}$.

[6] Writing the dipole's Hamiltonian $H_1(z) = H_F + V(z,t)$, let $z = z_0$ and consider a virtual displacement $z_0 \to z_0 + \Delta z$ of the external particle. We use stationary state perturbation theory to calculate the corresponding change in the ground state energy of the dipole. We have at $z = z_0$

$$H_1(z_0) \mid \phi_g(z_0) >= E_g(z_0) \mid \phi_g(z_0) > \tag{14}$$

and at $z = z_0 + \Delta z$, to first order in Δz

$$H_1(z_0 + \Delta z) \approx H_F + V(z_0) + \frac{\partial V}{\partial z}(z_0)\Delta z \equiv H_1(z_0) + \Delta V \tag{15}$$

$$(H_1(z_0)+\Delta V) \mid \phi_g(z_0)+\delta\phi_g >= (E_g(z_0)+\Delta E_g) \mid \phi_g(z_0)+\delta\phi_g > \tag{16}$$

subtracting (14) from (16), neglecting second order terms in Δ, δ, we obtain

$$\Delta E_g =< \phi_g \mid \Delta V \mid \phi_g >= g(t)\frac{\partial f}{\partial z}(z_0)\bar{\sigma}_3(z_0)\Delta z \tag{17}$$

where $\bar{\sigma}_3(z_0) =< \phi_g(z_0) \mid \sigma_3 \mid \phi_g(z_0) >$. Renaming $z_0 + \Delta z \equiv z_0$, $H_0 + \Delta V \equiv H_0$ and repeating the above, we finally obtain eq. (6) after a succession of such steps and summation.

[7] The distant wavepacket enclosed in the grounded Faraday cage does not contribute to the polarization. Denoting $\epsilon_n = \sqrt{\alpha_n^2 + \beta_n^2 g^2 f^2[z(2)]}$, the condition for the vanishing of the public potentials is

$$\frac{\beta_1^2}{\epsilon_1} - \frac{\beta_2^2}{\epsilon_2} = 0 \;\Rightarrow \beta_1^2\epsilon_2 - \beta_2^2\epsilon_1 = 0\,. \tag{18}$$

On the other hand, the Born Oppenheimer or private potential is $U_{BO}(z) = E_g^1(z) + E_{exc}^2(z)$. Thus $U_{BO}[z(2)] - U_{BO}[z(1)] = \epsilon_2 - \alpha_2 - [\epsilon_1 - \alpha_1]$ which in general is different from zero.

Captions for Figures

Fig. 1. The external particle is in a superposition of the wave packets ψ_1 and ψ_2, contained in the Faraday cages C_1, C_2 respectively. The dipole is at the origin.

Fig. 2. Electric AB Effect like interference experiment.